22nd NIST Computer Modeling Workshop
sponsored by RILEM and in cooperation with ASTM Committees C01 and C09

DATE and LOCATION

Wednesday July 20, 2011 to Friday July 22, 2011
Lecture Room B, Building 101
National Institute of Standards and Technology
Gaithersburg, Maryland 20899 USA

INSTRUCTORS

Jeff Bullard (coordinator), Dale Bentz, Edward Garboczi, Nicos Martys, Paul Stutzman, NIST
Materials and Construction Research Division
James Warren, NIST Center for Computational and Theoretical Materials Science
Barbara Lothenbach, EMPA
Jason Weiss, Purdue University
Rouzbeh Shahsavari, Rice University
Enrico Masoero, MJ Abdolhosseini Qomi, MIT

GENERAL DESCRIPTION

The workshop lectures will cover computational and experimental materials science of concrete topics, including simulation of microstructural development and prediction of physical properties. "Microstructure" ranges from nanometer to meter length scales, while physical properties include pressure-driven fluid flow, rheology, mechanical properties, neutron scattering, scanning electron microscopy, and various X-radiation probes like diffraction and tomography. Close cooperation between computation and experiment is crucial for making progress in the materials science of concrete and so is an emphasis of the workshop. The workshop will have a mix of tutorial lectures and short 15-minute talks by the participants describing their technical work. In addition, this year's workshop will also provide a tutorial for using the Virtual Cement and Concrete Testing Laboratory (eVCCTL) software.

WORKSHOP SCHEDULE

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<u>WEDNESDAY July 20, 2011   Lecture Room B, Administration Building</u>

9:30-9:45 Welcome and Orientation   Jeff Bullard

9:45-10:30 Lecture No. 1
Principles of modeling cement and concrete   Ed Garboczi

10:30-10:45 Break

10:45-11:45 Lecture No. 2   Paul Stutzman
Microstructure in portland cement paste and concrete

11:45-1:15 Lunch, NIST Cafeteria

1:15-2:15 Lecture No. 3   Jeff Bullard
Simulating early-age hydration of cement paste

2:15-2:30 Break

2:30-3:30 Lecture No. 4   Jason Weiss
Early-age properties of concrete

3:30-3:45 Break

3:45-5:00 Workshop Participants Presentations (5)
5:00 Bus leaves for Holiday Inn

8:30-9:30 Lecture No. 5   Barbara Lothenbach
Thermodynamic modeling of cement hydration

9:30-9:45 Break

9:45-12:00 Software Tutorial   Jeff Bullard
Using eVCCTL software for concrete education and research

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:15 Lecture No. 6   Dale Bentz
Sustainable concrete materials: experiments and modeling

2:15-2:30 Break

2:30-3:30 Lecture No. 7   Nicos Martys
Modeling rheological properties of fresh concrete

3:30-4:00 Workshop Participant Presentations (2)

4:00 Bus to NIST Center for Neutron Research (NCNR)

4:05-5:00 Tour of NCNR

5:00 Bus back to Building 101

8:30-9:00 Lecture No. 8   Jeff Bullard
Thermodynamic modeling and microstructure development

9:00-9:30 Lecture No. 9   E. Masoero
A novel Grand Canonical Monte Carlo approach to modeling cement setting

9:30-9:45 Break

                                                                             R. Shahsavari

9:45-10:45 Lecture No. 10
C-S-H texture from nanometers to micrometers

10:45-11:00 Break

11:00-11:30 Lecture No. 11   MJA Qomi
C-S-H and C-A-S-H under the nanoscope

11:30-1:00 Lunch, NIST Cafeteria

1:00-2:30 Lecture No. 15   James Warren
Phase field modeling and applications in materials science

2:30 Walk to Center for Nanoscale Science and Technology (CNST)

2:40-3:40 Tour of CNST

4:00-5:00 Workshop Participant Presentations (4)

5:00 Bus leaves for Holiday Inn

5:00 and 5:30 NIST Shuttle leaves for Shady Grove Metro to downtown Washington, DC

Registration

The list of workshop participants will be finalized by **June 30, 2011**, which is the application deadline. On-line registration is available at (http://www.nist.gov/el/building_materials/modeling-workshop.cfm).   The registration fee is $20.

Housing and Meals

A partial list of hotels near NIST is available on the workshop website. Many of these hotels offer shuttle services to and from NIST. Participants are also encouraged to use their favorite travel websites to search for special rates or other accommodations. Workshop participants are responsible for the costs of meals.

Getting to NIST

See the following web site for detailed information about getting to NIST (e.g., taxis, shuttles, restaurants) –http://www.nist.gov/public_affairs/visitor/visitor.htm.
If workshop participants land in Dulles International Airport, a taxi can be taken directly to the Gaithersburg Holiday Inn at a cost of about $70.00. Those persons flying into Reagan National Airport can take the Metro underground train directly to the Shady Grove stop in Gaithersburg (about $3-$6, depending on time of day—see signs in Airport station--Yellow line to Gallery Place, Red line to Shady Grove). A taxi may be taken from there to the Gaithersburg for about $15.00.

Alternatively, a taxi can be taken directly to the hotel from Reagan National for about $65.00. From Baltimore Washington International Airport, taxis cost about $90.00 to Gaithersburg. Shuttles are somewhat cheaper – see the airport web site for details. Driving directions to NIST are included on the NIST web site.

Security

All workshop attendees must have a picture I.D. with them to be able to enter the gates, either riding on the bus from Holiday Inn or by themselves. A U.S. driver's license or passport is fine. A temporary NIST badge will be given to you on your first entrance to NIST, which, along with your picture I.D., will allow entrance into NIST for the rest of the workshop. So don't throw it away! And please wear the NIST badge at all times while within NIST.

Note: Non-US citizens are required to give some additional information. You will see a place for this on the on-line registration.

Direct all questions to the Workshop coordinator:
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